Electronic Supplementary Material (ESI) for Physical Chemistry Chemical Physics

Supporting Information

On the chemical bonding feature in the boron containing compounds: a combined QTAIM / ELF topological analysis

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Table S1: Cartesian Coordinates (in Å) for [$(NHC)_2(B_2H_n)$, n=0,2 or 4] (§ III-1) optimized with B3LYP/TZVP

[$(NHC)_2(B_2H_4)$]; E = -662.0057679 a.u.

N	-2.622324323531	-0.775032635465	-1.077225380768
C	-1.790153576941	-0.860551296065	0.000000000000
N	-2.622324323531	-0.775032635465	1.077225380768
C	-3.939714408312	-0.623721234155	0.675586882215
C	-3.939714408312	-0.623721234155	-0.675586882215
B	-0.224145798013	-0.897075861172	0.000000000000
B	0.224014919806	0.897089824309	0.000000000000
C	1.790031205984	0.860327361762	0.000000000000
N	2.622180272860	0.774808816969	-1.077214248609
C	3.939613294754	0.623896100534	-0.675590462969
C	3.939613294754	0.623896100534	0.675590462969
N	2.622180272860	0.774808816969	1.077214248609
C	2.161768606810	0.787577983538	-2.455129366264
C	2.161768606810	0.787577983538	2.455129366264
C	-2.161942670634	-0.786794753176	2.455158871835
C	-2.161942670634	-0.786794753176	-2.455158871835
H	-0.185428900571	1.449145212796	1.005422056633
H	0.185435494373	-1.449027463976	1.005447349135
H	0.185435494373	-1.449027463976	-1.005447349135
H	-0.185428900571	1.449145212796	-1.005422056633
H	-4.748877416880	-0.534317476194	-1.377944512658
H	-4.748877416880	-0.534317476194	1.377944512658
H	4.748760826316	0.534384074212	-1.377949047048
H	4.748760826316	0.534384074212	1.377949047048
H	1.478002281915	-0.044305550576	-2.621135334386
H	1.639483175333	1.719533654634	-2.668730071834
H	3.024485228490	0.692037595228	-3.112456879356
H	3.024485228490	0.692037595228	3.112456879356
H	1.639483175332	1.719533654634	2.668730071834
H	1.478002281915	-0.044305550576	2.621135334386
H	-3.025336773070	-0.698241417455	3.112634274606
H	-1.633384236170	-1.715580153092	2.666984274666
H	-1.483677827101	0.049354231762	2.622756643197
H	-3.025336773070	-0.698241417455	-3.112634274606
H	-1.483677827101	0.049354231762	-2.622756643197
H	-1.633384236170	-1.715580153092	-2.666984274666

[$(NHC)_2(B_2H_2)$]; E = -660.7776267 a.u.

B	-0.639831550146	-0.486942961717	0.000000000000
B	0.639429153161	0.487652828300	0.000000000000
H	-0.575340540967	-1.687897033953	0.000000000000
H	0.574833496172	1.688599243308	0.000000000000
C	-2.123587370767	-0.058370759335	0.000000000000
N	-2.707684515444	1.190669210134	0.000000000000
C	-4.084630307814	1.094635088219	0.000000000000
C	-4.396099187193	-0.221133105202	0.000000000000

N	-3.206581292453	-0.919772441678	0.000000000000
C	2.123204794985	0.059172153998	0.000000000000
N	3.206181672236	0.920590986171	0.000000000000
C	4.395709852771	0.221962189389	0.000000000000
C	4.084256052502	-1.093813442144	0.000000000000
N	2.707312408993	-1.189856870285	0.000000000000
C	1.980669071848	-2.441683602401	0.000000000000
C	3.112366956834	2.367918950709	0.000000000000
C	-1.981062395807	2.442509769452	0.000000000000
C	-3.112807962725	-2.367105051649	0.000000000000
H	-4.718846523710	1.962923797893	0.000000000000
H	-5.352566160386	-0.712554538181	0.000000000000
H	4.718475229536	-1.962100573353	0.000000000000
H	5.352165929132	0.713399104638	0.000000000000
H	2.699091270540	-3.260175759037	0.000000000000
H	1.339017409066	-2.504402928097	0.879348252895
H	1.339017409066	-2.504402928097	-0.879348252895
H	4.120949885207	2.778755253031	0.000000000000
H	2.577459689059	2.716947674028	-0.883515678713
H	2.577459689059	2.716947674028	0.883515678713
H	-2.577919396921	-2.716157732583	-0.883516724301
H	-2.577919396921	-2.716157732583	0.883516724301
H	-4.121403615247	-2.777910856867	0.000000000000
H	-1.339416435172	2.505256565705	-0.879349132592
H	-2.699506883326	3.260982262452	0.000000000000
H	-1.339416435172	2.505256565705	0.879349132592

[$(NHC)_2(B_2)$]; E = -659. 5136785 a.u.

N	3.166534082968	-0.207666523633	0.693295919749
C	2.165892117979	0.446063301231	-0.000080055482
N	2.826452021969	1.441973094438	-0.693770449177
C	4.185393956984	1.392076493022	-0.433616055334
C	4.394950286767	0.375596828245	0.433099074633
B	0.713821414616	0.147097284843	0.000196055799
B	-0.713821414616	-0.147097284843	0.000196055799
C	-2.165892117979	-0.446063301231	-0.000080055482
N	-3.166534082968	0.207666523633	0.693295919749
C	-4.394950286767	-0.375596828245	0.433099074633
C	-4.185393956984	-1.392076493022	-0.433616055334
N	-2.826452021969	-1.441973094438	-0.693770449177
C	-2.910960798170	1.316023346875	1.586836340449
C	-2.153147982766	-2.359491219724	-1.586532509597
C	2.153147982766	2.359491219724	-1.586532509597
C	2.910960798170	-1.316023346875	1.586836340449
H	5.304685659365	0.018898871830	0.882150962996
H	4.879919324064	2.079255486809	-0.882969506063
H	-5.304685659365	-0.018898871830	0.882150962996
H	-4.879919324064	-2.079255486809	-0.882969506063
H	-3.855588938387	1.794044784008	1.843177703374
H	-2.413455371912	0.975608921439	2.498675991481

H	-2.253856603889	2.034098329828	1.092469419870
H	-2.833074657062	-3.170080244077	-1.845768763445
H	-1.827125438106	-1.849638521978	-2.496808285359
H	-1.267913424028	-2.762051712660	-1.090355843893
H	1.827125438106	1.849638521978	-2.496808285359
H	1.267913424028	2.762051712660	-1.090355843893
H	2.833074657062	3.170080244077	-1.845768763445
H	2.253856603889	-2.034098329828	1.092469419870
H	3.855588938387	-1.794044784008	1.843177703374
H	2.413455371912	-0.975608921439	2.498675991481

Table S2: Cartesian Coordinates (in Å) for ptB (§ III-2) optimized with B3LYP/Def2-SVP

E = -827.3234774 a.u.

B	0.533707	0.298187	0.479954
B	-0.519712	-0.308386	-0.531169
B	1.192606	-0.697448	-0.895197
B	-1.178612	0.687250	0.843981
H	0.874203	-1.337182	-1.865590
H	-0.860328	1.325525	1.815374
C	-2.688082	0.632165	0.469463
C	2.702077	-0.642364	-0.520678
H	-3.287629	0.534605	1.396079
H	3.301623	-0.544803	-1.447294
C	3.017160	0.404938	0.579670
C	-3.003166	-0.415136	-0.630885
H	3.732661	0.032691	1.344676
H	-3.718667	-0.042890	-1.395891
C	1.707703	0.764161	1.194690
C	-1.693708	-0.774360	-1.245905
H	1.680908	1.354785	2.115435
H	-1.666913	-1.364984	-2.166650
Si	3.922154	1.966247	-0.113118
Si	-3.230453	2.432444	-0.015698
Si	3.214444	-2.415903	0.081477
Si	-3.908159	-1.976446	0.061902
H	6.199169	2.350079	-1.089623
H	-5.463022	3.439725	-0.506675
H	6.248964	1.030930	0.103924
H	-5.632515	2.109719	0.664729
H	5.609582	0.732409	-1.530614
H	-5.423675	1.752852	-1.067498
H	4.628583	2.800202	2.151835
H	4.682976	4.107082	0.945733
H	3.120956	3.592248	1.627944
H	3.457257	3.625361	-1.921286

H	2.844583	2.022460	-2.388745
H	1.934003	3.014752	-1.224420
H	-2.813393	3.946217	-1.959107
H	-1.725372	3.767439	1.499772
H	-3.252935	4.624787	1.178576
H	-3.212519	3.286896	2.350856
H	-2.542996	2.246107	-2.422815
H	-1.309897	3.113756	-1.483214
C	-2.395650	2.984003	-1.617986
C	-2.812471	3.634545	1.383956
C	-5.110126	2.425606	-0.253302
C	2.946862	2.723200	-1.544268
C	4.103340	3.231535	1.283150
C	5.651503	1.469826	-0.712429
C	5.092951	-2.429404	0.330162
C	2.786920	-3.701284	-1.240334
C	2.355151	-2.854389	1.704642
H	5.419101	-1.720623	1.107775
H	5.623491	-2.174575	-0.602109
H	5.424371	-3.435614	0.638215
H	3.211994	-3.428378	-2.220590
H	3.194801	-4.688175	-0.963853
H	1.698359	-3.811005	-1.367590
H	2.752717	-3.804778	2.099228
H	2.507497	-2.078463	2.471297
H	1.268836	-2.972578	1.565727
C	-2.935897	-2.732715	1.495564
C	-4.086838	-3.242641	-1.333751
C	-5.639220	-1.481123	0.657197
H	-2.833785	-2.030681	2.338954
H	-1.923016	-3.026451	1.177725
H	-3.448334	-3.633460	1.873271
H	-3.103902	-3.600821	-1.679627
H	-4.663474	-4.119643	-0.994792
H	-4.614662	-2.813447	-2.201932
H	-6.190589	-2.363290	1.024401
H	-6.231725	-1.034554	-0.158601
H	-5.600074	-0.750411	1.481518

Table S3: Cartesian Coordinates (in Å) for [RuH2(η^2: η^2-H_2BMes)$PCy_3)_2$] (§ III-3) optimized with B3LYP/LanL2DZ.

E = - 1895.0938011a.u.

C	-0.819650	3.263304	-0.201051
C	-0.783237	4.119410	0.952159
C	-1.205669	5.460677	0.859054
H	-1.164234	6.091280	1.746180
C	-1.677812	6.009842	-0.348991

C	-1.704006	5.178156	-1.485928
H	-2.054819	5.587060	-2.432681
C	-1.285793	3.834116	-1.434276
C	-0.278521	3.633440	2.303918
H	-0.869151	2.788873	2.680450
H	-0.327846	4.437300	3.047504
H	0.761273	3.287526	2.248148
C	-1.345271	3.026496	-2.722963
H	-1.754592	3.630411	-3.541133
H	-1.971207	2.133344	-2.615021
H	-0.350012	2.676540	-3.027602
C	-2.161153	7.446994	-0.420277
H	-1.960516	7.888827	-1.404040
H	-1.677214	8.071786	0.340160
H	-3.246698	7.506087	-0.250953
C	3.458500	-0.330382	1.585329
H	3.380146	-1.381075	1.905994
C	2.698133	0.518392	2.636602
H	1.641174	0.229559	2.645540
H	2.735355	1.581899	2.352268
C	3.317165	0.347954	4.044272
H	2.779420	0.980773	4.765709
H	3.181365	-0.695113	4.373146
C	4.824158	0.692342	4.051413
H	4.950760	1.767096	3.842744
H	5.253382	0.508080	5.046822
C	5.585338	-0.124745	2.982517
H	5.560794	-1.191717	3.256285
H	6.643875	0.173744	2.958651
C	4.961269	0.055048	1.575232
H	5.521611	-0.544161	0.848107
H	5.074126	1.106830	1.275240
C	3.120715	-2.013506	-0.943227
H	2.540690	-2.017285	-1.878001
C	2.661248	-3.239337	-0.115313
H	3.219490	-3.277568	0.834067
H	1.599914	-3.136520	0.134786
C	2.909759	-4.556959	-0.889133
H	2.607123	-5.413535	-0.269101
H	2.271108	-4.572226	-1.786384
C	4.389756	-4.702445	-1.311812
H	5.013561	-4.822758	-0.411383
H	4.525719	-5.610809	-1.916693
C	4.870666	-3.461455	-2.098207
H	4.333601	-3.408855	-3.058612
H	5.940766	-3.553623	-2.336046
C	4.621443	-2.153835	-1.304126
H	5.224487	-2.183501	-0.385588
H	4.972438	-1.298152	-1.894836
C	3.472602	0.974886	-1.196005

H	4.545898	0.741791	-1.127933
C	3.041471	0.888066	-2.682411
H	3.237699	-0.114499	-3.086073
H	1.955170	1.046554	-2.746519
C	3.772160	1.941213	-3.551160
H	4.848982	1.707955	-3.576687
H	3.409198	1.878828	-4.587574
C	3.576245	3.372207	-3.001436
H	2.514775	3.653860	-3.088416
H	4.147939	4.092355	-3.604578
C	4.001600	3.457854	-1.519003
H	3.805234	4.465443	-1.125544
H	5.088191	3.289891	-1.442241
C	3.255576	2.410696	-0.657046
H	3.591925	2.488558	0.385285
H	2.181532	2.643694	-0.661177
C	-2.086425	-3.033229	0.409991
H	-1.217686	-3.144593	1.075358
C	-3.301572	-3.707655	1.099309
H	-3.535709	-3.221702	2.053993
H	-4.196122	-3.620830	0.467096
C	-3.013539	-5.208522	1.364197
H	-2.188370	-5.291635	2.089450
H	-3.893953	-5.676801	1.829056
C	-2.628606	-5.961378	0.070921
H	-3.497440	-5.986348	-0.606701
H	-2.375477	-7.006247	0.301977
C	-1.447780	-5.267216	-0.644523
H	-0.542729	-5.349440	-0.022047
H	-1.227902	-5.775408	-1.594850
C	-1.748789	-3.772779	-0.908684
H	-2.602481	-3.706204	-1.599982
H	-0.891484	-3.293839	-1.396474
C	-3.108739	-0.539679	1.761553
H	-4.019502	-1.156267	1.796770
C	-2.280828	-0.811817	3.043639
H	-1.994583	-1.870843	3.102682
H	-1.343323	-0.241586	2.987990
C	-3.060683	-0.411594	4.318661
H	-2.433822	-0.586887	5.205350
H	-3.948722	-1.056032	4.423321
C	-3.508468	1.066467	4.264133
H	-4.102897	1.318636	5.154268
H	-2.617800	1.714970	4.281843
C	-4.322080	1.351821	2.981815
H	-4.584434	2.418385	2.926477
H	-5.270348	0.791665	3.024912
C	-3.547915	0.943462	1.703463
H	-4.186964	1.126065	0.828905
H	-2.663538	1.584521	1.589501

C	-3.355165	-0.663648	-1.232624
H	-3.483223	0.421446	-1.090056
C	-4.757980	-1.316750	-1.154433
H	-4.668069	-2.401746	-1.308013
H	-5.207346	-1.167968	-0.163093
C	-5.697020	-0.737647	-2.242057
H	-5.866498	0.332385	-2.041852
H	-6.678488	-1.231419	-2.188549
C	-5.093343	-0.901366	-3.655687
H	-5.031471	-1.973935	-3.900553
H	-5.753213	-0.441058	-4.405123
C	-3.679142	-0.280312	-3.733410
H	-3.757948	0.811625	-3.608772
H	-3.242335	-0.455224	-4.727508
C	-2.742230	-0.856059	-2.643451
H	-1.756574	-0.377629	-2.688301
H	-2.582402	-1.923930	-2.843442
P	2.551130	-0.347049	-0.131273
P	-2.124250	-1.099627	0.195164
Ru	0.118141	-0.213747	-0.023578
B	-0.350164	1.784734	-0.123734
H	0.368098	-1.338019	1.114102
H	0.215670	-1.452162	-1.050364
H	-0.143005	1.183507	-1.237096
H	0.010746	1.348160	1.019514

Table S4: Cartesian Coordinates (in Å) for [$Cr(CO)_5(\eta^1$-$BH_3.PH_3)$] (§ III-4) optimized with B3LYP/TZVP & SDD.

E = -1023.7651397 a.u.

C	-0.007343884402	0.028667202342	-0.001807142126
O	-0.011672915165	0.043741101498	1.144710344527
Cr	0.028917115516	0.002380621092	-1.907207991767
C	1.889057359043	0.015701353497	-1.871319228524
O	3.038380817788	0.024132263447	-1.844166287280
C	-0.002880627968	-1.910763324351	-1.888258430770
O	-0.009329300354	-3.055036536752	-1.874006501314
C	0.050789664398	-0.024836036351	-3.825969855045
O	0.099982677620	-0.040480458985	-4.967845080214
C	-0.029064762742	1.914557711487	-1.942559562523
O	-0.051379000392	3.058611394574	-1.960791010547
B	-2.720102521849	-0.023719325151	-2.500537709289
P	-4.230512091987	-0.002369884556	-1.241392259585
H	-1.798614448546	-0.007714188043	-1.673910724370
H	-2.856865975473	0.980318003378	-3.137241204386
H	-2.853050073318	-1.051787647422	-3.098625682057
H	-4.347812529535	-1.073332385258	-0.329204104626
H	-5.506397589523	-0.017701138963	-1.842628572875
H	-4.353406911450	1.103805278869	-0.373020998356

Table S5: Cartesian Coordinates (in Å) for [$Cr(CO)_4(\eta^2$-$B_2H_4.2PMe_3$)] (§ III-4) optimized with B3LYP/LanL2DZ.

E = -844.1726467 a.u.

Cr	-1.533451488081	-0.003253034062	-0.003159371517
C	-2.792847865364	0.939653441748	0.941729761764
C	-2.789684712506	-0.947897951398	-0.950850566924
C	-1.603344543672	-1.328197271416	1.326126105949
C	-1.601168021972	1.323185372559	-1.330764600207
H	-0.355091890232	-0.954335850295	-1.084516873748
H	-0.360284815895	0.948187519274	1.082653579401
B	0.764064840930	-0.546401549944	-0.671601377825
B	0.761075756277	0.545530141963	0.670514186225
H	1.333069642995	-0.203248165933	-1.687746922499
H	1.329857390755	0.203969362971	1.687375059740
P	1.693094586942	-2.273497834672	-0.251703078220
P	1.682150986951	2.278095092734	0.254039705974
C	1.237950873586	-3.681282315303	-1.409444358901
C	3.550724231902	-2.089210101462	-0.459761337899
C	1.508529066547	-2.998714371610	1.469285483246
C	1.197897338963	3.687237484028	1.398129713739
C	3.538202940518	2.110723772590	0.488986702263
C	1.515944871930	2.992826686577	-1.473251871367
H	1.823742785593	-4.581603705286	-1.193939185156
H	0.172684781862	-3.906616691822	-1.297304601470
H	1.416116968879	-3.368871030041	-2.443390907629
H	4.061876868354	-3.045009008745	-0.301990773234
H	3.765834493164	-1.724683618736	-1.469051439655
H	3.923008977320	-1.359490087726	0.266233121670
H	2.209668505750	-3.828884492361	1.608755211414
H	1.709494115889	-2.217718460884	2.207864115845
H	0.487594442428	-3.356762686524	1.622073238224
H	2.211172138058	3.828922637631	-1.606791628295
H	1.735216879038	2.209881652507	-2.204561450244
H	0.493992121533	3.340197309678	-1.642905462049
H	4.043512453302	3.069939500559	0.333241299427
H	3.742165465296	1.753116971625	1.503033669311
H	3.926725724534	1.380401217862	-0.227877566493
H	1.779728141732	4.591342775576	1.187862256553
H	0.132699938294	3.903339635611	1.268380465006
H	1.362236570237	3.380600482526	2.436097761072
O	-1.716919904535	2.157226424172	-2.167556293204
O	-1.720231739009	-2.157407074912	2.167430934494
O	-3.584150989845	-1.578961202405	-1.572043298036
O	-3.587474394747	1.569072645896	1.564463830946